

We claim:

1. A method for obtaining a statistical classifier for classifying microorganisms of unknown species into known species, comprising:
 - (a) obtaining a plurality of magnetic resonance spectra of each of a plurality of different species of microorganisms whose species is known;
 - (b) locating a plurality of maximally discriminatory subregions in the magnetic resonance spectra obtained; and
 - (c) cross-validating the spectra by selecting a first portion of the spectra from each species, developing linear discriminant analysis classifiers from the first portion of the spectra from each species, and validating the remainder of the spectra from each species using the classifiers from the first portion of the spectra from each species to obtain optimized linear discriminant analysis coefficients and classifier spectra for each of the known species of microorganisms, which coefficients and classifier spectra can be used to determine the species of microorganisms whose species are unknown.
2. The method of claim 1, further comprising the step of repeating step (c) a plurality of times, each time selecting as the first portion of the spectra a different portion of the spectra from the species, to obtain a different set of optimized linear discriminant analysis coefficients for the species, and obtaining a weighted average of the linear discriminant analysis coefficients to obtain final classifier spectra.

5

3. The method of claim 1, wherein the step of cross-validating the spectra comprises cross validating the spectra by randomly selecting about half of the spectra.
4. The method of claim 2, wherein the step of repeating step (c) a plurality of times comprises repeating step (c) about 1000 times.
- 10 5. The method of claim 1, further including the steps of obtaining a plurality of classifier spectra independently, and aggregating the results of the independent classifiers to obtain a consensus diagnosis.
6. The method of claim 1, wherein the microorganisms include bacteria.
7. The method of claim 6, wherein the bacteria includes the species of *Staphylococcus aureus* and *Staphylococcus epidermidis*.
- 15 8. The method of claim 6, wherein the bacteria includes the species of *Enterococcus faecalis*, *Enterococcus casseliflavus* and *Enterococcus gallinarum*.
9. The method of claim 6, wherein the bacteria includes the species of *Streptococcus pneumoniae*, *Streptococcus pyogenes* and *Streptococcus agalactiae*.
- 20 10. The method of claim 1, wherein the microorganisms include fungi.
11. The method of claim 10, wherein the fungi includes pathogenic yeasts.
12. The method of claim 11, wherein the pathogenic yeasts include *Candida albicans*, *Candida parapsilosis*, *Candida tropicalis*, *Candida krusei*, and *Candida glabrata*.
13. The method of claim 11, wherein the pathogenic yeasts include *Cryptococcus* varieties.
- 25 14. The method of claim 13, wherein the *Cryptococcus* varieties include *neoformans* and *gattii*.

5 15. The method of claim 1, wherein the plurality of magnetic resonance spectra of each different species is at least 10.

16. The method of claim 1, wherein the plurality of magnetic resonance spectra of each different species is at least 30.

17. The method of claim 1, wherein the microorganisms include cultured bacterial infections.

10 18. The method of claim 1, wherein the microorganisms include specimens from a mammal containing bacterial infections.

19. A method for determining the species of a microorganism of unknown species, comprising:

Obtaining magnetic resonance spectra of the microorganism of unknown species,
15 and comparing the spectra obtained with a species classifier, said classifier having been obtained by

(a) obtaining a plurality of magnetic resonance spectra of each of a plurality of different species of microorganisms whose species is known;

20 (b) locating a plurality of maximally discriminatory subregions in the magnetic resonance spectra obtained; and

(c) cross-validating the spectra by selecting a first portion of the spectra from each species, developing linear discriminant analysis classifiers from the first portion of the spectra from each species, and validating the remainder of the spectra from each species using the classifiers from the first portion of the spectra from each species to obtain optimized linear discriminant analysis coefficients and classifier

25

5 spectra for each of the known species of microorganisms; and
selecting, as the species of the unknown species of microorganism,
the microorganism whose spectra has the closest match to the spectra
of the unknown microorganism species.

10 20. The method of claim 19, wherein the steps of obtaining the classifier further comprises
the step of repeating step (c) a plurality of times, each time selecting as the first portion of
the spectra a different portion of the spectra from the species, to obtain a different set of
optimized linear discriminant analysis coefficients for the species, and obtaining a
weighted average of the linear discriminant analysis coefficients to obtain final classifier
spectra.

15 21. The method of claim 19, wherein the step of cross-validating the spectra comprises cross
validating the spectra by randomly selecting about half of the spectra.

22. The method of claim 20, wherein the step of repeating step (c) a plurality of times
comprises repeating step (c) about 1000 times.

20 23. The method of claim 19, further including the steps of obtaining a plurality of classifier
spectra independently, and aggregating the results of the independent classifiers to obtain
a consensus diagnosis.

24. The method of claim 19, wherein the microorganisms include bacteria.

25 25. The method of claim 24, wherein the bacteria includes the species of *Staphylococcus*
aureus and *Staphylococcus epidermidis*.

26. The method of claim 24, wherein the bacteria includes the species of *Enterococcus*
faecalis, *Enterococcus casseliflavus* and *Enterococcus gallinarum*.

- 5 27. The method of claim 6, wherein the bacteria includes the species of *Streptococcus pneumoniae*, *Streptococcus pyogenes* and *Streptococcus agalactiae*.
28. The method of claim 1, wherein the microorganisms include fungi.
29. The method of claim 28, wherein the fungi includes pathogenic yeasts.
30. The method of claim 29, wherein the pathogenic yeasts include *Candida albicans*,
10 *Candida parapsilosis*, *Candida tropicalis*, *Candida krusei*, and *Candida glabrata*.
31. The method of claim 29, wherein the pathogenic yeasts include *Cryptococcus* varieties.
32. The method of claim 31, wherein the *Cryptococcus* varieties include *neoformans* and *gattli*.
33. The method of claim 19, wherein the plurality of magnetic resonance spectra of each
15 different species is at least 10.
34. The method of claim 19, wherein the plurality of magnetic resonance spectra of each different species is at least 30.
35. The method of claim 19, wherein the microorganisms include cultured bacterial infections.
- 20 36. The method of claim 19, wherein the microorganisms include specimens from a mammal containing bacterial infections.
37. A statistical classifier for classifying microorganisms of unknown species into known species, comprising:
- 25 (a) a spectrometer for obtaining a plurality of magnetic resonance spectra of each of a plurality of different species of microorganisms whose species is known;

- 5 (b) a locator for locating a plurality of maximally discriminatory subregions in
the magnetic resonance spectra obtained; and
- (c) a cross-validator for cross-validating the spectra by selecting a first portion
of the spectra from each species, developing linear discriminant analysis
classifiers from the first portion of the spectra from each species, and
10 validating the remainder of the spectra from each species using the classifiers
from the first portion of the spectra from each species to obtain optimized
linear discriminant analysis coefficients and classifier spectra for each of the
known species of microorganisms, which coefficients and classifier spectra
can be used to determine the species of microorganisms whose species are
15 unknown.
38. The classifier of claim 37, wherein the cross-validator repeats step (c) a plurality of times,
each time selecting as the first portion of the spectra a different portion of the spectra
from the species, to obtain a different set of optimized linear discriminant analysis
coefficients for the species, and obtaining a weighted average of the linear discriminant
20 analysis coefficients to obtain final classifier spectra.
39. The classifier of claim 37, wherein the cross-validator cross validates the spectra by
randomly selecting about half of the spectra.
40. The classifier of claim 38, wherein the classifier repeats step (c) about 1000 times.
41. The classifier of claim 37, wherein the classifier obtains a plurality of classifier spectra
25 independently, and aggregates the results of the independent classifiers to obtain a
consensus diagnosis.
42. The classifier of claim 37, wherein the microorganisms includes bacteria.

- 5 43. The classifier of claim 42, wherein the bacteria includes the species of *Staphylococcus aureus* and *Staphylococcus epidermidis*.
44. The classifier of claim 42, wherein the bacteria includes the species of *Enterococcus faecalis*, *Enterococcus casseliflavus* and *Enterococcus gallinarum*.
45. The classifier of claim 42, wherein the bacteria includes the species of *Streptococcus pneumoniae*, *Streptococcus pyogenes* and *Streptococcus agalactiae*.
- 10 46. The classifier of claim 37, wherein the microorganisms include fungi.
47. The classifier of claim 46, wherein the fungi includes pathogenic yeasts.
48. The classifier of claim 47, wherein the pathogenic yeasts include *Candida albicans*, *Candida parapsilosis*, *Candida tropicalis*, *Candida krusei*, and *Candida glabrata*.
- 15 49. The classifier of claim 47, wherein the pathogenic yeasts include *Cryptococcus* varieties.
50. The classifier of claim 49, wherein the *Cryptococcus* varieties include *neoformans* and *gattli*.
51. The classifier of claim 37, wherein the plurality of magnetic resonance spectra of each different species is at least 10.
- 20 52. The classifier of claim 37, wherein the plurality of magnetic resonance spectra of each different species is at least 30.
53. The classifier of claim 1, wherein the microorganisms include cultured bacterial infections.
54. The classifier of claim 1, wherein the microorganisms include specimens from a mammal
- 25 containing bacterial infections.